

L Number	Hits	Search Text	DB	Time stamp
1	1815	(436/173,85,86,).CCLS.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/23 18:19
2	517	((436/173,85,86,).CCLS.) and NMR	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/23 18:19
-	45	NMR with integral\$2 with mixture\$2	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/18 16:43
-	21	(NMR with integral\$2 with mixture\$2) and (polymer\$2 or protein\$2)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/14 15:28
-	776	(NMR or "nuclear magnetic resonance") with integral\$2	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/14 15:32
-	50	((NMR or "nuclear magnetic resonance") with integral\$2 ) and (mixture\$2 with integral\$3)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/14 15:34
-	25	((((NMR or "nuclear magnetic resonance") with integral\$2 ) and (mixture\$2 with integral\$3)) and (polymer\$2 or biopolymer\$3 or protein\$3))	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/18 16:44
-	4722	(NMR or "nuclear magnetic resonance") and integral\$2 and mixture\$2 and (polymer\$2 or biopolymer\$3 or protein\$3)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/18 18:46
-	1989	((NMR or "nuclear magnetic resonance") and integral\$2 and mixture\$2 and (polymer\$2 or biopolymer\$3 or protein\$3)) and quantitat\$4	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/18 16:45
-	568	((((NMR or "nuclear magnetic resonance") and integral\$2 and mixture\$2 and (polymer\$2 or biopolymer\$3 or protein\$3)) and quantitat\$4) and (mixture\$2 near4 (polymer\$2 or biopolymer\$3 or protein\$3))	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/18 16:48
-	2	((((NMR or "nuclear magnetic resonance") and integral\$2 and mixture\$2 and (polymer\$2 or biopolymer\$3 or protein\$3)) and quantitat\$4) and (mixture\$2 near4 (polymer\$2 or biopolymer\$3 or protein\$3))) and (mixtur\$3 near6 integral\$2)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/18 16:49
-	992	(NMR or "nuclear magnetic") with proteins	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/18 18:47
-	225	((NMR or "nuclear magnetic") with proteins) and integral\$2	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/18 18:48
-	6	((NMR or "nuclear magnetic") with proteins) with integral\$2	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/01/18 18:48

10065163

FILE 'CAPLUS' ENTERED AT 15:42:20 ON 14 JAN 2004

L1 308 (NMR OR "NUCLEAR MAGNETIC") (S) INTEGRAL?

L2 4 L1 AND (MIXTURE? (S) (POLYMER? OR BIOPOLYMER? OR PROTEIN?))

L3 1 (POLYMER? (6A) MIXTURE?) AND ((NMR OR "NUCLEAR MAGNETIC") (S) INTEGRAL?)

L2 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:5879 CAPLUS

DOCUMENT NUMBER: 86:5879

TITLE: Application of the NMR technique to the quantitative analysis of aldehyde groups in the presence of the epoxide ring

AUTHOR(S): Rybczyk, Marzenna; Wasielewska, Anna

CORPORATE SOURCE: Zak. Polim., PAN, Zabrze, Pol.

SOURCE: Chemia Analityczna (Warsaw, Poland) (1976), 21(3), 631-6

CODEN: CANWAJ; ISSN: 0009-2223

DOCUMENT TYPE: Journal

LANGUAGE: Polish

AB Two methods of determination of aldehyde groups in the presence of epoxide groups in the reaction medium during polymerization of <SYM97>-methylglycidaldehyde (I) [52788-68-8] have been described. The calculations are based on a comparison of the integral intensity of the NMR signal corresponding to aldehyde protons with integral intensity corresponding to protons of a weighted standard. In the first method a known amount of a standard compound (nitrobenzene) was added to a weighted sample of the reaction mixture consisting of I, its polymerization products, and catalyst and the integral intensity of the nitrobenzene proton signals was taken as reference. The second, more direct method, is based on the fact that the amount of methyl protons corresponding to I, its polymerization products, solvent and catalyst is known and constant in the reaction mixture during polymerization so that the integral intensity of signals corresponding to methyl protons may be utilized as standard

L3 ANSWER 1 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative nuclear magnetic resonance analysis of solid formoterol fumarate and its dihydrate

L3 ANSWER 2 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Process for quantitative determination by NMR of at least one compound in a mixture

L3 ANSWER 3 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative on-line high-resolution NMR spectroscopy in process engineering applications

L3 ANSWER 4 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative analysis of mixtures of 1- and 2-isopropylnaphthalene and corresponding oxidation products by <sup>1</sup>H-NMR spectroscopy

L3 ANSWER 5 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Complex polymer mixture analysis by on-line LC(GPC)-NMR

L3 ANSWER 6 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative NMR Spectroscopy of Complex Liquid Mixtures: Methods and Results for Chemical Equilibria in Formaldehyde-Water-Methanol at Temperatures up to 383 K

L3 ANSWER 7 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Biocatalytic Polymerization of p-Cresol: An in-Situ NMR Approach To Understand the Coupling Mechanism

L3 ANSWER 8 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative determination of aliphatic hydrocarbon compounds by 2D NMR

L3 ANSWER 9 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Regiochemistry of Cleavage of Monosubstituted Oxiranes by Phosphorochloridites. Enantiomeric Composition of Oxiranes by <sup>31</sup>P NMR Spectral Data

L3 ANSWER 10 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Application of Quantitative Artificial Neural Network Analysis to 2D NMR Spectra of Hydrocarbon Mixtures

L3 ANSWER 11 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Proximity Effects in Monolayer Films: Kinetic Analysis of Amide Bond Formation at the Air-Water Interface Using <sup>1</sup>H NMR Spectroscopy

L3 ANSWER 12 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Regioselectivity in nitration of biphenyl derivatives

L3 ANSWER 13 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Complex polymer mixture analysis by LC(GPC)-NMR

L3 ANSWER 14 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Theoretical investigations of NMR chemical shieldings on the ALPON catalyst system

L3 ANSWER 15 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Multivariate analysis and quantitation of <sup>17</sup>O-nuclear magnetic resonance in primary alcohol mixtures

L3 ANSWER 16 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative determination of methylcyclohexanone mixtures using <sup>13</sup>C NMR spectroscopy

L3 ANSWER 17 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI <sup>1</sup>H NMR quantitative analysis of acetates, long chain fatty acids and phenols in a humus sample of municipal solid wastes after methane fermentation

L3 ANSWER 18 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI The quantitative method of the blend which includes the surfactant

L3 ANSWER 19 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative <sup>13</sup>C NMR assay and assignment of mixtures from lipase digestion of propane-1,2-diol dibutyrate

L3 ANSWER 20 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Direct qualitative and quantitative analysis of triterpenes using <sup>13</sup>C NMR spectroscopy exemplified by dichloromethanic extracts of cork

L3 ANSWER 21 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Determination of polar organic pollutants in aqueous samples of former ammunition sites in Lower Saxony by means of HPLC/photodiode array detection (HPLC/PDA) and proton nuclear magnetic resonance spectroscopy (<sup>1</sup>H-NMR)

L3 ANSWER 22 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Regiospecific analysis of natural mixtures of triglycerides using quantitative <sup>13</sup>C-nuclear magnetic resonance of acyl chain carbonyl carbons

- L3 ANSWER 23 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Classification and quantitation of  $^1\text{H}$  NMR spectra of alditols binary mixtures using artificial neural networks
- L3 ANSWER 24 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Additions of carbon nucleophiles to acyclic imine complexes of the chiral rhenium Lewis acid [ $(\text{C}_5\text{H}_5)_2\text{Re}(\text{NO})(\text{PPh}_3)_2$ ] $^+$ : controlling factors in 1,3-asymmetric induction and syntheses of non-racemic organic amines
- L3 ANSWER 25 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Direct qualitative and quantitative analysis of carbohydrate mixtures using  $^{13}\text{C}$  NMR spectroscopy: application to honey
- L3 ANSWER 26 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Determination of phenytoin, phenobarbitone and methyl phenobarbitone in combination
- L3 ANSWER 27 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Online  $^1\text{H}$ -NMR to facilitate tube preparation in SNIF-NMR analysis
- L3 ANSWER 28 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Highly sensitive spectroscopic detection of chiral molecular structures by  $^{77}\text{Se}$  NMR spectroscopy
- L3 ANSWER 29 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Determination of the composition of delavirdine mesylate polymorph and pseudopolymorph mixtures using  $^{13}\text{C}$  CP/MAS NMR
- L3 ANSWER 30 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Kinetics of cocondensation between phenol and urea through formaldehyde. I. Pseudo-first-order reaction of monomethylphenol and urea
- L3 ANSWER 31 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Characterization of hydrogenated derivatives of methyl- and dimethyldicyclopentadiene isomers by gas chromatography-mass spectrometry and carbon- $^{13}$  nuclear magnetic resonance spectroscopy
- L3 ANSWER 32 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Application of computer-assisted  $^{13}\text{C}$  NMR spectrometry for separation and determination of heptane isomers in the feedstocks of cyclohexane used in purification process
- L3 ANSWER 33 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Quantitation of bilobalide and ginkgolides A, B, C and J by means of nuclear magnetic resonance spectroscopy
- L3 ANSWER 34 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Quantitation and structure elucidation of the positional isomers in a triacylglycerol mixture using proton and carbon one- and two-dimensional NMR
- L3 ANSWER 35 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Response of the phosphatidylcholine headgroup to membrane surface charge in ternary mixtures of neutral, cationic, and anionic lipids: A deuterium NMR study
- L3 ANSWER 36 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI A route to quantitative carbon- $^{13}$  NMR analysis of multicomponent polyesters
- L3 ANSWER 37 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Characterization of methyl derivatives of cyclopentadiene monomer and dimer by carbon- $^{13}$  NMR spectroscopy

- L3 ANSWER 38 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Computer-assisted carbon-13 NMR spectroscopic identification and determination of chlorohydrins in reaction mixtures formed during manufacture of glycerol
- L3 ANSWER 39 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Analysis of mixed lipid extracts using proton NMR spectra
- L3 ANSWER 40 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Determination of C-7 isomer distribution in commercial feedstocks by GC-matrix isolation-FT-IR-MS
- L3 ANSWER 41 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Phosphorus-31 NMR spectroscopy for labile hydrogen group analysis: toward quantitation of phenols in a coal condensate
- L3 ANSWER 42 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Modeling of hydrogen transfer in coal hydroliquefaction. 4. The reaction of benzyl phenyl ether with four hydroaromatic solvents at 300°C
- L3 ANSWER 43 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Application of high-resolution proton NMR spectroscopy for quantitative determination of o-, m- and p-chlorotoluenes in mixtures
- L3 ANSWER 44 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Quantitation of the relative amounts of anhydrous carbamazepine (C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O) and carbamazepine dihydrate (C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O·2H<sub>2</sub>O) in a mixture by solid-state nuclear magnetic resonance (NMR)
- L3 ANSWER 45 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Carbon-13 MAS NMR spectroscopy of inorganic and biogenic carbonates
- L3 ANSWER 46 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Advances in the field of analysis of phenol mixtures
- L3 ANSWER 47 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Multicomponent quantitative analysis using second-order nonbilinear data: theory and simulations
- L3 ANSWER 48 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Analysis of phospholipids by phosphorus-31 NMR
- L3 ANSWER 49 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI (Vinylxy)chlorocyclotetraphosphazenes. The use of two dimensional phosphorus-31 NMR spectroscopy in phosphazene chemistry
- L3 ANSWER 50 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Application of Kirkwood-Buff theory to free energies of transfer of electrolytes from one solvent to another
- L3 ANSWER 51 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI Determination of competitive reaction mixture content by proton NMR
- L3 ANSWER 52 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI A comparative spectroscopic investigation of 3 pseudopolymorphs of testosterone using solid-state IR and high-resolution solid-state NMR
- L3 ANSWER 53 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
TI NMR-spectroscopy of carbon-14-labeled amino acid mixtures. V. Computer analysis of spectra
- L3 ANSWER 54 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Complete assignment of the carbon-13 NMR spectra of the ring forms of digitoxose by DEPT spectrum editing and two-dimensional carbon-proton chemical shift correlation spectroscopy

L3 ANSWER 55 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Application of NMR to phase diagram study - isothermal phase diagram of the sodium chloride-ammonium chloride-water system by sodium-23 and nitrogen-14 NMR quantitative method

L3 ANSWER 56 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative analysis of pyrrolizidine alkaloid mixtures from *Senecio vulgaris* by carbon-13 nuclear magnetic resonance spectroscopy

L3 ANSWER 57 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI (Vinyl)oxychlorocyclotetraphosphazenes. The use of two-dimensional phosphorus-31 NMR spectroscopy in phosphazene chemistry

L3 ANSWER 58 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Identification of mixture components in organic waste materials by carbon-13 nuclear magnetic resonance

L3 ANSWER 59 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Identification of organic mixture components without separation: quantitative and edited carbon-13 nuclear magnetic resonance spectrometry data for analysis of petroleum distillates

L3 ANSWER 60 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative NMR assay for aspirin, phenacetin, and caffeine mixtures with 1,3,5-trioxane as internal standard

L3 ANSWER 61 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative analysis of phospholipids by phosphorus-31 NMR

L3 ANSWER 62 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative determination of o-, m- and p-xylenes by <sup>13</sup>C-NMR spectroscopy

L3 ANSWER 63 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Analysis of gas chromatography-mass spectrometry library search results with edited and quantitative <sup>13</sup>C nuclear magnetic resonance spectra

L3 ANSWER 64 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Analysis of hexanol mixture by the chromatographic method

L3 ANSWER 65 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative proton Fourier transform nuclear magnetic resonance spectroscopic analysis of mixtures of pyrrolizidine alkaloids from *Senecio vulgaris*

L3 ANSWER 66 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Spectroscopic data processing. NMR1 software and its applications in chemistry and biophysics

L3 ANSWER 67 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Determination of gentamicin C major components by NMR

L3 ANSWER 68 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative analysis by pulsed Fourier transform proton nuclear magnetic resonance

L3 ANSWER 69 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Reorientation and transalkylation reactions of isotopically labeled toluene, ethylbenzene, and propylbenzene

L3 ANSWER 70 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

- TI Determination of the enantiomeric purity of <SYM97>-tocopherol by carbon-13 NMR spectroscopy  
L3 ANSWER 71 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Quantitative NMR determination of citric acids in mixtures  
L3 ANSWER 72 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI The effects of T1 and NOE considerations in quantitative applications of carbon-13 NMR to the analysis of complex hydrocarbon mixtures  
L3 ANSWER 73 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Determination of protonated and quaternary carbons in H-coal liquids from quaternary carbon suppressed and nonsuppressed CMR spectra  
L3 ANSWER 74 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI New methods for analysis of lignite liquefaction products  
L3 ANSWER 75 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Use of a lanthanide shift reagent in the analysis of isomer ratio  
L3 ANSWER 76 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Carbon-13 nuclear magnetic resonance spectra of E-silyl-alkenes  
L3 ANSWER 77 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Quantitative analysis of <SYM97>,<SYM97>,<SYM97>,2,4-pentachlorotoluene and <SYM97>,<SYM97>,<SYM97>,2,5-pentachlorotoluene mixtures by carbon-13 Fourier transform nuclear magnetic resonance spectrometry  
L3 ANSWER 78 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Quantitative analysis by pulsed Fourier transform (Ft) <sup>13</sup>C NMR. II. Quantitative analysis of normal paraffins, carbonyl containing compounds and substituted benzene isomer mixture  
L3 ANSWER 79 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Simultaneous determination of vitamins B1 and B6 by nuclear magnetic resonance spectrometry  
L3 ANSWER 80 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Approach to the quantitative analysis of di-sec-butylamine stereoisomeric mixtures by means of NMR  
L3 ANSWER 81 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Quantitative analysis of mixtures by carbon-13 nuclear magnetic resonance spectrometry  
L3 ANSWER 82 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI An enzyme-P.M.R. spectroscopic determination of the enantiomers of galactose  
L3 ANSWER 83 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Simultaneous on-line computer analysis of multicomponent systems by quantitative NMR spectroscopy  
L3 ANSWER 84 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Carbon-13-NMR study of the mutarotation equilibriums of D-fructose and 1-amino-1-deoxy-D-fructose derivatives (Amadori combinations)  
L3 ANSWER 85 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Quantitative analysis of meso and racemic 2,3-diaminobutane mixtures by nuclear magnetic resonance spectroscopy  
L3 ANSWER 86 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative NMR analysis of a four-component mixture of phenylglycine derivatives

L3 ANSWER 87 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative determination of relative isomeric ratios of 1H- and 2H-tetrazole-1-acetic acids and their ester analogs by nuclear magnetic resonance spectroscopy

L3 ANSWER 88 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Isotropic analysis of mixtures of deuterated ethanols, C<sub>2</sub>H<sub>5</sub>-n-D<sub>n</sub>OH

L3 ANSWER 89 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI NMR quantitative analysis of quinidine in mixtures of quinidine and hydroquinidine

L3 ANSWER 90 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Application of carbon-13 NMR to the characterization of petroleum fractions

L3 ANSWER 91 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Quantitative analysis by phosphorus-31 nuclear magnetic resonance spectrometry

L3 ANSWER 92 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Photo-rearrangements of methyl indole-1-acetate, indole-1-acetamide, and methyl indoline-1-acetate

L3 ANSWER 93 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Nuclear magnetic resonance applied to the quantitative analysis of organic substances

L3 ANSWER 94 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Analysis of hydroxy steroids by 19F-NMR spectroscopy. Determination of structure and quantitative analyses of hydroxy steroid mixtures in the microgram range

L3 ANSWER 95 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Drug analysis by nuclear magnetic resonance. 3. Qualitative and quantitative analysis of analgesics

L3 ANSWER 96 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Method based on quantitative NMR spectrometry for the determination of alpha-olefinic content in multicomponent samples

L3 ANSWER 97 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Use of spin decoupling to obtain quantitative data in olefin analysis by N.M.R.

L3 ANSWER 98 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI Application of nuclear magnetic resonance to quantitative analysis of mixtures of organic peroxides, hydroperoxides, and alcohols

L3 ANSWER 99 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI <SYM98>-Methylation of alcohols. I. The synthesis of hydratropic and 2-methyl-2-cyclohexylethyl alcohols

L3 ANSWER 100 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

TI <SYM98>-Unsaturated alcohols obtained by thermal condensation of. formol with olefins

L3 ANSWER 2 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:680293 CAPLUS

DOCUMENT NUMBER: 139:206664

TITLE: Process for quantitative determination by NMR of at least one compound in a mixture

INVENTOR(S): Libes, Francois



PATENT ASSIGNEE(S): Fr.  
SOURCE: Fr. Demande, 19 pp.  
CODEN: FRXXBL  
DOCUMENT TYPE: Patent  
LANGUAGE: French  
PATENT NO. KIND DATE APPLICATION NO. DATE

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FR 2836553 A1 20030829 FR 2002-2375 20020225  
WO 2003073120 A2 20030904 WO 2003-FR596 20030224  
PRIORITY APPLN. INFO.: FR 2002-2375 A 20020225

AB The present invention has as an aim a process of quant. determination by NMR of spins in fast exchange between at least two different compartments of a mixture, in particular in physicochem., the determination being carried out via two consecutive phases of measurement carried out each by application to a volume of sample to analyze sequences of impulsions. The process is characterized in that the 1st phase of measurement is carried out with an authorized relaxation time (T1) appreciably allowing a total relaxation of the spins of all the compartments present, and in which the 2nd phase of measurement is carried out with a relaxation time authorized (s) (t2) permitting partial relaxation of at least a category of spins, i.e. pertaining to the one of the compartments.

REFERENCE COUNT: 4

L3 ANSWER 13 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:206049 CAPLUS

TITLE: Complex polymer mixture analysis by LC(GPC)-NMR

AUTHOR(S): Wu, Jian; Beshah, Kebede

CORPORATE SOURCE: Analytical and Computational Technology Center, Rohm and Haas Company, Bristol, PA, 19007, USA

SOURCE: Abstracts of Papers - American Chemical Society  
(2001), 221st, POLY-289

CODEN: ACSRAL; ISSN: 0065-7727

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal; Meeting Abstract

LANGUAGE: English

AB We have recently explored the application of online LC-NMR and GPC-NMR methods to quant. determine polymer compns. in a mixture or simply as a function of mol. weight distribution. Such a powerful tool has not been fully exploited for polymer characterization due to strong solvent signals in NMR. In this study, we have successfully applied the bipolar gradient pulses stimulated echo sequence (BPPSTE) to suppress solvent and small mol. impurity signals, based on the different diffusion property between polymers and small mols. The lower the mol. weight of the species, the higher the diffusion coefficient, hence the faster the signal decays with BPPSTE NMR. Using a reverse-phase C-18 column and acetonitrile/THF solvent gradient, we have examined polybutadiene, poly(Me methacrylate) (pMMA), polystyrene and poly(Bu acrylate) (pBA) polymer mixts. and have completely determined the structure and blockiness (monomer sequences) of various copolymers in the mixture. With the online GPC-NMR, we were able to determine the complete composition and blockiness of

pMMA, pBA and polystyrene mixts. at various mol. wts. The GPC-NMR method proved to be an excellent approach to examine the chemical composition and microstructure of polymers as a function of the distribution of mol. weight. The potential application of LC-NMR on other polymer mixts. will also be discussed.

L3 ANSWER 15 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:169182 CAPLUS

DOCUMENT NUMBER: 132:273128

TITLE: "Multivariate analysis and quantitation of  $^{17}\text{O}$ -nuclear magnetic resonance in primary alcohol mixtures"

AUTHOR(S): *Alam, M. K.; Alam, T. M.*

CORPORATE SOURCE: Materials and Process Computation and Modeling  
Department, Sandia National Laboratories, Albuquerque, NM, USA

SOURCE: **Spectrochimica Acta, Part A: Molecular and Biomolecular  
Spectroscopy (2000), 56A(4), 729-738**

CODEN: SAMCAS; ISSN: 1386-1425

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Multivariate techniques were used to address the quantification of  $^{17}\text{O}$ -NMR spectra for primary alc. mixts. Due to highly overlapping resonances, quant. spectral evaluation using standard integration and deconvolution techniques proved difficult. Multivariate evaluation of the  $^{17}\text{O}$ -NMR spectral data obtained for 26 mixts. of five primary alcs. demonstrated that obtaining information about spectral overlap and interferences allowed the development of more accurate models. Initial partial least squares (PLS) models developed for the  $^{17}\text{O}$ -NMR data collected from the primary alc. mixts. resulted in very poor precision, with signal overlap between the different chemical species suspected of being the primary contributor to the error. To directly evaluate the question of spectral overlap in these alc. mixts., net analyte signal (NAS) analyses were performed. The NAS results indicate that alcs. with similar chain lengths produced severely overlapping  $^{17}\text{O}$ -NMR resonances. Grouping the alcs. based on chain length allowed more accurate and robust calibration models to be developed.

REFERENCE COUNT: 19

L3 ANSWER 19 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:248547 CAPLUS

DOCUMENT NUMBER: 131:55688

TITLE: Quantitative  $^{13}\text{C}$  NMR assay and assignment of mixtures from lipase digestion of propane-1,2-diol dibutyrate

AUTHOR(S): O'Connor, Charmian J.; Barton, Richard H.

CORPORATE SOURCE: Department of Chemistry, The University of Auckland,  
Auckland, N. Z.

SOURCE: Australian Journal of Chemistry (1999), 52(2), 123-127

CODEN: AJCHAS; ISSN: 0004-9425

PUBLISHER: CSIRO Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

AB <sup>13</sup>C NMR spectra were obtained at 50 and 100 MHz for mixts. of propanediol, propane-1,2-diol dibutyrate, propane-1,2-diol 1-butyrate and propane-1,2-diol 2-butyrate in CDCl<sub>3</sub>. Distortionless enhancement by polarization transfer (DEPT) and two-dimensional <sup>13</sup>C-<sup>1</sup>H correlation spectroscopy were used to confirm shift assignments. Spectra for the 1- and 2-monoesters showed strongly different inductive effects due to the position of the butyryl chain. These expts. demonstrate the desirability of using <sup>13</sup>C NMR rather than <sup>1</sup>H NMR spectroscopy in quant. speciation of acylated diol complex hydrolysis mixts. REFERENCE COUNT: 7

L3 ANSWER 20 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:193472 CAPLUS

DOCUMENT NUMBER: 130:352444

TITLE: "Direct qualitative and quantitative analysis of triterpenes using <sup>13</sup>C NMR spectroscopy exemplified by dichloromethanic extracts of cork"

AUTHOR(S): *Castola, Vincent; Bighelli, Ange; Casanova, Joseph*

CORPORATE SOURCE: Universite de Corse, Equipe Chimie et Biomasse, URA CNRS 2053, Ajaccio, 20000, Fr.

SOURCE: Applied Spectroscopy (1999), 53(3), 344-350

CODEN: APSPA4; ISSN: 0003-7028

PUBLISHER: Society for Applied Spectroscopy

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe a methodol. which allows identification and quantitation of individual triterpenes in natural mixts., using the computer-aided anal. of their <sup>13</sup>C NMR spectra, without previous separation. The anal. procedure was validated on artificial mixts. and applied to authentic exts. of cork. Identification of triterpenes was possible with the use of either reference spectra recorded in our laboratory or literature data.

REFERENCE COUNT: 39

L3 ANSWER 22 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:408587 CAPLUS

DOCUMENT NUMBER: 129:69071

TITLE: Regiospecific analysis of natural mixtures of triglycerides using quantitative <sup>13</sup>C-nuclear magnetic resonance of acyl chain carbonyl carbons

AUTHOR(S): Vlahov, Giovanna

CORPORATE SOURCE: Istituto Sperimentale per la Elaiotecnica, Pescara, 65013, Italy

SOURCE: Magnetic Resonance in Chemistry (1998), 36(5), 359-362

CODEN: MRCHEG; ISSN: 0749-1581

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB High-resolution <sup>13</sup>C-NMR spectroscopy of the carbonyl carbons of triglyceride acyl chains was used as a quant. method for regiospecific anal. of triglyceride fraction of vegetable oils of different botanical origins. The carbonyl carbon resonances of saturated,

oleyl and linoleyl chains were baseline resolved. Moreover, the chains attached at the 1,3-position were shifted by 0.4 ppm at higher frequencies than those of the corresponding chains attached at the 2-position. This quant. NMR method was adopted after demonstrating that proton decoupling affected the carbonyl intensities to the same extent, no significant differences being found among the NOE factors of different acyl chains. The proton-decoupled spectra were measured for quant. purposes with full NOE enhancement. As a result, the spectrum signal-to-noise ratios were significantly improved in shorter experiment times. REFERENCE COUNT: 20

L3 ANSWER 23 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:136103 CAPLUS

DOCUMENT NUMBER: 128:188084

TITLE: "Classification and quantitation of  $^1\text{H}$  NMR spectra of alditols binary mixtures using artificial neural networks"

AUTHOR(S): *Amendolia, Salvator Roberto; Doppiu, Angelino; Ganadu, Maria Luisa; Lubinu, Giuseppe*

CORPORATE SOURCE: Istituto di Matematica e Fisica, Dipartimento di Chimica, Sassari, 07100, Italy

SOURCE: **Analytical Chemistry (1998), 70(7), 1249-1254**

CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A pattern recognition method based on artificial neural networks (ANNs) to analyze and quantify the components of six alditol binary mixts. is presented. This method is suitable to classify the spectra of the 15 mixts. obtained from the six alditols and to produce quant. ests. of the component concns. The system is user-friendly and is helpful in solving the problem of greatly overlapping signals, often encountered in NMR spectroscopy of carbohydrates. A classification ANN uses 200 intensity values of the  $^1\text{H}$  NMR spectrum in the range 3.5-4 ppm. When the correct mixture is identified, the quantification is solved by assigning a specific ANN to each mixture. These ANNs use the same 200 values of the spectrum and output the values of the two concns. The error in the ANN responses was studied, and a method is developed to estimate the accuracy in determining the concns. The networks' abilities to recognize previously unseen mixts. are tested. When the classification ANN (trained on the 15 binary mixts.) is exposed to complex (i.e., more than binary) mixts. of the six known alditols, it successfully identifies the components if their min. concentration is 10%. Given the precision of the results and the small number of errors reported, probably the method can should be used in all fields in which the recognition and quantification of components are necessary.

REFERENCE COUNT: 25

L3 ANSWER 25 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:35533 CAPLUS

DOCUMENT NUMBER: 128:139850

TITLE: "Direct qualitative and quantitative analysis of carbohydrate mixtures using  $^{13}\text{C}$  NMR spectroscopy: application to honey"

AUTHOR(S): *Mazzoni, Vanina; Bradesi, Pascale; Tomi, Felix; Casanova, Joseph*  
CORPORATE SOURCE: Equipe Chimie et Biomasse, Universite de Corse,  
CRES-URA CNRS 2053, Ajaccio, 20000, Fr.

SOURCE: **Magnetic Resonance in Chemistry (1997), 35(Spec. Issue), S81-S90**

CODEN: MRCHEG; ISSN: 0749-1581

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A method is described which allows the identification of individual carbohydrates of multi-component artificial mixts. using the computer-aided anal. of their  $^{13}\text{C}$  NMR spectra, without previous separation. Quantitation of mono-, di- and trisaccharides was carried out after improvement of the exptl. procedure and using an internal standard. The procedure was then applied to authentic honeys of different floral types, harvested in Corsica (France). Several oligosaccharides (identification of some of these is not easy by chromatog. techniques) were observed at levels ranging from 0.4 to 3.3%. In addition, the fructose/glucose ratio, which has an influence on crystallization, was easily obtainable.

REFERENCE COUNT: 51

L3 ANSWER 36 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:130063 CAPLUS

DOCUMENT NUMBER: 116:130063

TITLE: A route to quantitative carbon-13 NMR analysis of multicomponent polyesters

AUTHOR(S): Hvilsted, Soeren

CORPORATE SOURCE: Mater. Dep., Risoe Natl. Lab., Roskilde, DK-4000, Den.

SOURCE: Makromolekulare Chemie, Macromolecular Symposia (1991), 52(Eur. Symp. Polym. Spectrosc., 9th, 1990), 199-208

CODEN: MCMSES; ISSN: 0258-0322

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A protocol for quant. sequential  $^{13}\text{C}$  NMR anal. is developed for polyesters composed of trimethylolpropane (I), neopentyl glycol (II), and adipic and isophthalic acids. I-centered structural models with Me adipate and isophthalate branches in all possible combinations are synthesized and purified. A detailed  $^{13}\text{N}$  NMR investigation of the models unequivocally allows the identification of the I polyester structural sequences through the quaternary I carbon multiplicity. Spin-lattice relaxation times of model quaternary I carbons are in the 2.3-5.2 s range, depending on the size of the specific model. This relaxation behavior defines the exptl. conditions for obtaining the quant. assessment of all polyester polyol structural sequences based on quaternary I and II carbons. The special case dealt with here addnl. centers all acid moieties between polyols in triads and thus makes quant. detns. of all polyester constituents possible.

L3 ANSWER 43 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:604229 CAPLUS

DOCUMENT NUMBER: 113:204229

TITLE: "Application of high-resolution proton NMR spectroscopy for quantitative determination of o-, m- and p-chlorotoluenes in mixtures"

AUTHOR(S): *Husain, Sajid; Sastry, L. Ramachandra; Rao, R. Nageswara*  
CORPORATE SOURCE: Indian Inst. Chem. Technol., Hyderabad, 500 007, India  
SOURCE: **Research and Industry (1990), 35(2), 86-90**  
CODEN: RSIDAO; ISSN: 0034-513X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A simple, specific and rapid quant.  $^1\text{H}$  NMR method is developed for simultaneous determination of o-, m- and p-chlorotoluenes in mixts. Spectra are recorded in a diamagnetic anisotropic solvent such as benzene- $d_6$  containing 4-bromoacetophenone as an internal standard. The acetyl proton resonance for the standard at  $\delta$  1.95 ppm is well separated from those Me resonances of o-, m- and p-chlorotoluenes which are at  $\delta$  2.14, 1.88 and 1.91 ppm, resp. Peak areas of the Me resonances are compared for quant. estimation of each isomer in mixts. Average percent recoveries of o-, m- and p-chlorotoluenes are 98.5, 97.7 and 98.9 with standard deviations of 0.7, 0.8, and 0.7, resp. This method is applied to the analyses of reaction mixts. obtained by chlorination of toluene.

L3 ANSWER 47 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:508304 CAPLUS

DOCUMENT NUMBER: 111:108304

TITLE: "Multicomponent quantitative analysis using second-order nonbilinear data: theory and simulations"

AUTHOR(S): *Wilson, Bruce E.; Lindberg, Walter; Kowalski, Bruce R.*

CORPORATE SOURCE: Dep. Chem., Univ. Washington, Seattle, WA, 98195, USA

SOURCE: **Journal of the American Chemical Society (1989), 111(11), 3797-804**

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The application of rank annihilation to a class of instrument generating data which can be classified as second-order nonbilinear is described. This method permits determining the concentration of an analyte of interest even in the presence of spectral interferences unknown and unaccounted for during calibration. The primary difficulty in applying rank annihilation to nonbilinear data is that multiple, different concentration ests. are obtained; it is shown that, for two-dimensional mass spectrometry and absolute value mode two-dimensional NMR spectroscopy, the correct concentration estimate should be the smallest of those obtained. The method provides a back-estimate of the calibration matrix, which can be used as an indication of the precision of the resulting concentration estimate, as well as a diagnostic for the presence of matrix effects between the calibration and unknown samples. In this paper, the theory and motivation for rank annihilation is presented, and the application to nonbilinear data is presented using computer simulations and a test system consisting of 2D J-coupled NMR spectra (COSY) of six sugars in  $\text{D}_2\text{O}$ .

L3 ANSWER 53 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:550636 CAPLUS

DOCUMENT NUMBER: 107:150636

TITLE: NMR-spectroscopy of carbon-14-labeled amino acid mixtures. V. Computer analysis of spectra

AUTHOR(S): Panov, V. P.; Dubrovin, V. I.; Tarabakin, S. V.; Smetanina, T. A.

CORPORATE SOURCE: Vses. Nauchno-Issled. Inst. Tekhnol. Krovezamenitelei Gorm. Prep., Moscow, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1987), 21(7), 877-81

CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Possible use of program ROBAND is described for the qual. and computer quant. NMR anal. of  $^{13}\text{C}$ -labeled multicomponent biol. mixts. (particularly amino acids) obtained via enzyme treatment of organs and the animal tissues. The automated system for collection, storage and processing data allows identification of the signal in the NMR spectra, identification of the components in the mixture, selection of anal. signals, resolution of complex contains, calcn. of the concentration of each component, and evaluation of the exptl. deviations. Block diagram of ROBAND is given and some related aspects are discussed.

L3 ANSWER 59 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:575562 CAPLUS

DOCUMENT NUMBER: 105:175562

TITLE: "Identification of organic mixture components without separation: quantitative and edited carbon-13 nuclear magnetic resonance spectrometry data for analysis of petroleum distillates"

AUTHOR(S): *Laude, David A., Jr.; Wilkins, Charles L.*

CORPORATE SOURCE: Dep. Chem., Univ. California, Riverside, CA, 92521, USA

SOURCE: **Analytical Chemistry (1986), 58(13), 2820-4**

CODEN: ANCHAM; ISSN: 0003-2700

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A method for the anal. of unknown mixts. which incorporates unique features of quant. and edited  $^{13}\text{C}$ -NMR is described. Chromatog. separation and subsequent identification by match with a spectroscopic data base spectrum is not required for quant. anal. of the components. Instead, equivalent information is obtained by creating subspectra from resonances with equivalent peak areas within a quant. NMR spectrum. Identification is accomplished by comparison of edited spectra with multiplicity data derived directly from the chemical structure of potential components. Anal. of petroleum distillates within the class of low-boiling (C5-7) hydrocarbon compds. is considered. A 207-component library is created and utilized in the anal. of 2 fractions for which 7 and 14 compds. are successfully identified.

L3 ANSWER 60 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:485276 CAPLUS

DOCUMENT NUMBER: 105:85276

TITLE: Quantitative NMR assay for aspirin, phenacetin, and caffeine mixtures with 1,3,5,-trioxane as internal standard

AUTHOR(S): Eberhart, Suzanne Thomson; Hatzis, Alexander; Rothchild, Robert  
CORPORATE SOURCE: John Jay Coll. Crim. Justice, City Univ. New York, New  
York, NY, 10019-1199, USA  
SOURCE: Journal of Pharmaceutical and Biomedical Analysis (1986), 4(2), 147-54  
CODEN: JPBADA; ISSN: 0731-7085

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The method using NMR for determining aspirin [50-78-2], phenacetin [62-44-2] and caffeine [58-08-2] (APC) mixts. was improved by the use of 1,3,5-trioxane [110-88-3] as an internal standard. The trioxane absorption occurs in a peak-free region of the spectrum and produces no interferences with any of the analytes. Compared to the original method with caffeine as an external standard, the present method appears to offer better accuracy and precision. Relative standard deviations were: aspirin, 1.0%; phenacetin, 0.8%; and caffeine 1.8%, for known standard mixts. Coupling consts.,  $1J_{13CH}$ , were determined for the Me groups of aspirin and caffeine and for the trioxane methylene group to clarify potential  $^{13}C$  satellite interferences.

L3 ANSWER 66 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:166812 CAPLUS

DOCUMENT NUMBER: 100:166812

TITLE: Spectroscopic data processing. NMR1 software and its applications in chemistry and biophysics

AUTHOR(S): Dumoulin, C. L.; Levy, G. C.

CORPORATE SOURCE: Dep. Chem., Syracuse Univ., Syracuse, NY, 13210, USA

SOURCE: Journal of Molecular Structure (1984), 113, 299-310

CODEN: JMOSB4; ISSN: 0022-2860

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The NMR1 software system (previously known as ORACLE) is a large modular FORTRAN 77 program for reduction of spectroscopic data from Fourier transform NMR expts., although the program is applicable to other types of spectroscopy. NMR1 features include: (1) implementation of powerful algorithms for optimization of data content; (2) routines for high accuracy quantitation of spectral features, including quant. separation of overlapping lines; (3) versatile output routines including color graphics and multi-format hard copy; (4) extensive user prompting and automation control. NMR1 is being used in a variety of chemical and biol. applications. Examples include quantitation of metabolic NMR spectra, anal. of  $^{13}C$  NMR of double stranded DNA, and quant. anal. of mixts. of organic compds.

L3 ANSWER 68 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1983:568763 CAPLUS

DOCUMENT NUMBER: 99:168763

TITLE: Quantitative analysis by pulsed Fourier transform proton nuclear magnetic resonance

AUTHOR(S): Peng, Pu; Lu, Wanzhen

CORPORATE SOURCE: Res. Inst. Pet. Process., Peop. Rep. China



SOURCE: Fenxi Huaxue (1983), 11(7), 552-4

CODEN: FHHHDT; ISSN: 0253-3820

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB A proton Fourier-transform NMR method is described for quant. anal. of mixts. with overlapping peaks and exptl. conditions are discussed in detail. The accuracy and precision of the method are illustrated with ethylbenzene and a typical gasoline sample. The relative standard deviations are <5% usually.

L3 ANSWER 71 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:154880 CAPLUS

DOCUMENT NUMBER: 94:154880

TITLE: Quantitative NMR determination of citric acids in mixtures

AUTHOR(S): Krivdin, L. B.; Chekareva, T. G.; Sakharovskii, V. G.; Romanova, I. B.

CORPORATE SOURCE: Inst. Biochem. Physiol. Microorg., Pushchino, USSR

SOURCE: Zhurnal Analiticheskoi Khimii (1981), 36(2), 357-63

CODEN: ZAKHA8; ISSN: 0044-4502

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB A high resolution NMR method is developed for the determination of citric acids in the culture filtrate of a microbial culture. The pH of the medium should be maintained <2.0. The method gives reproducible results and allows the simultaneous determination of citric acid [77-92-9], D-isocitric acid [30810-51-6], and D-isocitric acid lactone [19427-08-8].

L3 ANSWER 72 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:106151 CAPLUS

DOCUMENT NUMBER: 94:106151

TITLE: The effects of T1 and NOE considerations in quantitative applications of carbon-13 NMR to the analysis of complex hydrocarbon mixtures

AUTHOR(S) Alger, Terry D.; Pugmire, Ronald J.; Hamill, W. David, Jr.; Grant, David M.

CORPORATE SOURCE: Dep. Chem., Univ. Utah, Salt Lake City, UT, 84112, USA

SOURCE: Preprints of Papers - American Chemical Society, Division of Fuel Chemistry (1979), 24(2), 334-8

CODEN: ACFPAI; ISSN: 0569-3772

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Spin lattice relaxation times (T1) and Nuclear Overhauser Effect (NOE) were determined for naphthalene [91-20-3], Tetralin [119-64-2], acenaphthene [83-32-9], pyrene [129-00-0], symhexahydropyrene [1732-13-4], phenanthrene [85-01-8], 1,2,3,4,5,6,7,8-octahydrophenanthrene [5325-97-3], xanthone [90-47-1], and phenyloctane [2189-60-8]. These compds. represent many moieties occurring in coal liqs. The T1 and NOE values thus obtained provide valuable information on relaxation process, range of values expected, and details of mol. motion.

L3 ANSWER 78 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:54094 CAPLUS

DOCUMENT NUMBER: 90:54094

TITLE: "Quantitative analysis by pulsed Fourier transform (Ft)  $^{13}\text{C}$  NMR. II. Quantitative analysis of normal paraffins, carbonyl containing compounds and substituted benzene isomer mixture"

AUTHOR(S): Yamazaki, Mitsuru; Usami, Takao; Yanada, Shigeo; Takeuchi, Tsugio

CORPORATE SOURCE: Sch. Pharm., Hokuriku Univ., Kanazawa, Japan

SOURCE: **Nippon Kagaku Kaishi (1978), (11), 1509-14**

CODEN: NKAJB8; ISSN: 0369-4577

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB In order to apply pulse FT  $^{13}\text{C}$  NMR spectrometry to quant. anal., the quant. relationships between  $^{13}\text{C}$  NMR signal area intensity and number of resonating nuclei were investigated.  $\text{CH}_2$  carbon signal area intensity ratios (S.A.R) of (C-3 or higher carbon/C-2 carbon) in normal paraffins approached theor. ratios with increasing pulse delay (PD) and with decreasing pulse width (PW). In the case of tetradecane, the proportional relationship between S.A.R. and theor. ratio held with relative error 10% under  $\text{PW} = 20$   $\mu\text{s}$  and  $\text{PD} = 5$  s.  $^{13}\text{C}$  signal area intensity and signal-to-noise ratio (S/N) of carbonyl C in acetone-Me acetate mixts. were greatly influenced by PD and PW. The relative error for the determination of acetone in acetone-Me acetate mixts. was 3% under  $\text{PD} = 5$ -15 s and  $\text{PW} = 60$   $\mu\text{s}$ . The relative content of each component in an o-, m- and p-tolyl acetate mixture was determined by measuring the signal area intensity ratio of the ring C bonded to the OAc group or Me group and the carbonyl C in the OAc group. The relative error was approx. 6% under  $\text{PD} = 15$  s and  $\text{PW} = 60$   $\mu\text{s}$ .

L3 ANSWER 81 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:593305 CAPLUS

DOCUMENT NUMBER: 87:193305

TITLE: "Quantitative analysis of mixtures by carbon-13 nuclear magnetic resonance spectrometry"

AUTHOR(S): Mareci, Thomas H.; Scott, Katherine Nasfay

CORPORATE SOURCE: VA Hosp., Gainesville, FL, USA

SOURCE: **Analytical Chemistry (1977), 49(14), 2130-6**

CODEN: ANCHAM; ISSN: 0003-2700

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Results for quant. anal. of mixts. by  $^{13}\text{C}$  NMR, without nuclear Overhauser enhancement suppression, are presented. Two systems which are not simple isomeric mixts. are considered. Mixts. of 2 steroids, 3 $\alpha$ -acetoxy- and 3 $\beta$ -chlorocholesterol, and mixts. of 2 aromatic acids, 3,4-dihydroxyphenylpropionic and 3,4-dimethoxyphenylacetic acid, were quantified in varying concns. from 2 to 98 mol% with an average root mean square error of 1.6%. Spin-lattice relaxation times, effective transverse relaxation times, and nuclear Overhauser enhancements for these systems were determined. Based on these values, criteria were developed for the selection of resonances to be compared to yield accurate results.

L3 ANSWER 86 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1976:416620 CAPLUS  
DOCUMENT NUMBER: 85:16620  
TITLE: "Quantitative NMR analysis of a four-component mixture of phenylglycine derivatives"  
AUTHOR(S): *Warren, R. J.; Zarembo, J. E.; Staiger, D. B.; Post, A.*  
CORPORATE SOURCE: Smith Kline and French Lab., Philadelphia, PA, USA  
SOURCE: **Journal of Pharmaceutical Sciences (1976), 65(5), 738-40**  
CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A rapid, accurate, and precise NMR anal. method for the anal. of phenylglycine, dihydrophenylglycine, tetrahydrophenylglycine, and cyclohexylglycine in combination with each other was developed. The method is based on the integration of the NMR signal characteristic of each component relative to the signal from tetramethylammonium bromide, which is added as an internal standard. No prior separation of the 4 components is required.

L3 ANSWER 89 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1973:483500 CAPLUS  
DOCUMENT NUMBER: 79:83500  
TITLE: NMR quantitative analysis of quinidine in mixtures of quinidine and hydroquinidine  
AUTHOR(S): *Huynh Ngoc Tho; Sirois, Gerard*  
CORPORATE SOURCE: Fac. Pharm., Univ. Montreal, Montreal, QC, Can.  
SOURCE: **Journal of Pharmaceutical Sciences (1973), 62(8), 1334-6**  
CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A new procedure for the rapid quant. anal. of quinidine in mixts. of quinidine and hydroquinidine is described. The method is based upon measurement of the NMR spectrum of these compds. in CDCl<sub>3</sub>, using 2,3,5-tribromothiophene as an internal standard. The signal chosen is from the vinyl group of quinidine. The great advantage of this procedure is that it permits the determination of the percentage of hydroquinidine in com. bulk quinidine.

L3 ANSWER 90 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1973:161741 CAPLUS  
DOCUMENT NUMBER: 78:161741  
TITLE: Application of carbon-13 NMR to the characterization of petroleum fractions  
AUTHOR(S): *Clutter, D. R.; Petrakis, L.; Stenger, R. L.; Jensen, R. K.; Lett, R. G.*  
CORPORATE SOURCE: Gulf Res. and Dev. Co., Pittsburgh, PA, USA  
SOURCE: **Preprints - American Chemical Society, Division of Petroleum Chemistry (1971), 16(3), A97-A109**  
CODEN: ACPCAT; ISSN: 0569-3799

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The unique advantage of this technique is the focusing on the C skeleton of the many and complex structures of petroleum fractions. A discussion is presented on the potential, advantages, and problems of the C-13 NMR technique. Since C-13 NMR is a quant. measure of types of C present, true aromaticities were determined for pure compds., synthetic mixts., gas oils, and feedstocks. Chemical shifts were presented to show the possibility of determining specific compound types in various fractions. The possibility of using C-13 NMR for quick but often unequivocal 'fingerprintings' was also presented.

L3 ANSWER 91 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1973:92180 CAPLUS

DOCUMENT NUMBER: 78:92180

TITLE: Quantitative analysis by phosphorus-31 nuclear magnetic resonance spectrometry

AUTHOR(S): Colson, James G.; Marr, David H.

CORPORATE SOURCE: Res. Cent., Hooker Chem. Corp., Grand Island, NY, USA

SOURCE: Analytical Chemistry (1973), 45(2), 370-1

CODEN: ANCHAM; ISSN: 0003-2700

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The usefulness of <sup>31</sup>P NMR spectrometry in quant. anal. is demonstrated by anal. of mixts. of hydroxymethylphosphine derivs. and mixed Na thiophosphates. The previous use of the method for the anal. of condensed phosphates (M. M. Crutchfield et al., 1962) is also described briefly.

L3 ANSWER 96 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1970:38680 CAPLUS

DOCUMENT NUMBER: 72:38680

TITLE: Method based on quantitative NMR spectrometry for the determination of alpha-olefinic content in multicomponent samples

AUTHOR(S): Manjarrez, Armando; Esparza C., Maria de J.

CORPORATE SOURCE: Inst. Mex. Petrol., Mex.

SOURCE: Revista del Instituto Mexicano del Petroleo (1969), 1(3), 64-9

CODEN: RVMPAX; ISSN: 0538-1428

DOCUMENT TYPE: Journal

LANGUAGE: Spanish

AB Olefins of the CH<sub>2</sub>:CHR and CH<sub>2</sub>:CR<sub>2</sub> types in mixts. with other olefins and aromatics were determined by NMR at 60 and 100 MHz at 37°, by using 10% Me<sub>4</sub>Si in CCl<sub>4</sub> as a calibration standard and dioxane as an internal standard

L3 ANSWER 98 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1969:93006 CAPLUS

DOCUMENT NUMBER: 70:93006

TITLE: Application of nuclear magnetic resonance to quantitative analysis of mixtures of organic peroxides, hydroperoxides, and alcohols

AUTHOR(S): Ward, George Anthony; Mair, Robert D.

CORPORATE SOURCE: Res. Dep., Hercules Inc., Wilmington, DE, USA

SOURCE: Analytical Chemistry (1969), 41(3), 538-40

CODEN: ANCHAM; ISSN: 0003-2700

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The quant. N.M.R. anal. of peroxy compds. was studied briefly. Chemical shifts of the  $\alpha$ -protons are presented for RO<sub>2</sub>R, RO<sub>2</sub>H, and ROH (R = tert-Bu, 2-(p-toluy1)-2-propyl, 2-(p-isopropylphenyl)-2-propyl, 2-(p-chlorophenyl)-2-propyl, 2-(3,4-dichlorophenyl)-2-propyl, and 2-phenyl-2-propyl). The chemical shifts of the  $\beta$ -protons in R1O<sub>2</sub>H and R1OH (R1 = Pr, Bu, iso-Bu, n-octyl, and n-nonyl) are presented also. tert-BuO<sub>2</sub>H mixts. with 25.0, 50.0, 75.0, and 90.0% tert-BuOH were analyzed in replicate to contain  $25.2 \pm 0.6$ ,  $50.8 \pm 0.1$ ,  $72.4 \pm 0.7$ , and  $88.2 \pm 0.6\%$  tert-BuOH. In general, the relative error is 3% and the relative standard deviation  $<3\%$  for mixts. of peroxy compds. in which the N.M.R. peaks are separated by  $>0.8$  Hz. Apparently, the detection limit for the minor component in binary mixts. of peroxy compds. is 2-3%.